

=> fil reg

FILE 'REGISTRY' ENTERED AT 07:34:47 ON 24 FEB 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 FEB 2005 HIGHEST RN 836595-43-8

DICTIONARY FILE UPDATES: 23 FEB 2005 HIGHEST RN 836595-43-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

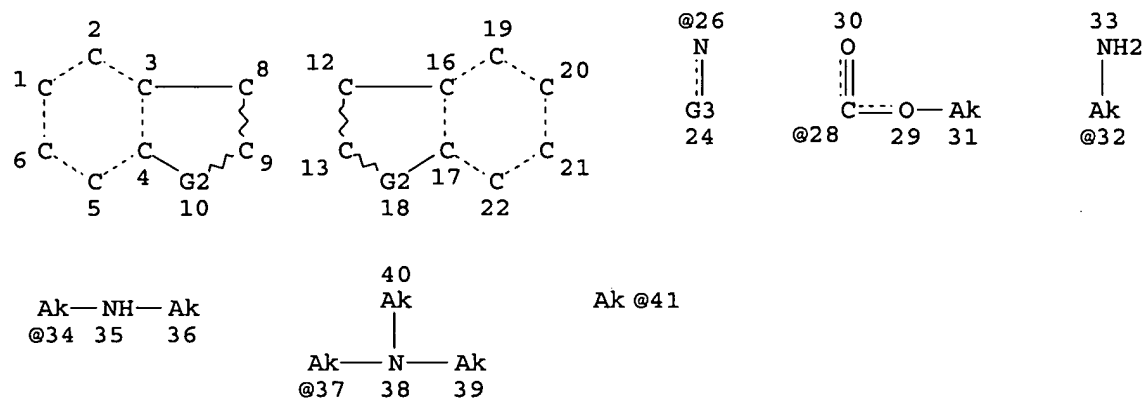
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> => d que l19

L14 STR



VAR G2=NH/26

VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 31

CONNECT IS E2 RC AT 32

CONNECT IS E2 RC AT 34

CONNECT IS E1 RC AT 36

CONNECT IS E2 RC AT 37

CONNECT IS E1 RC AT 39

CONNECT IS E1 RC AT 40

CONNECT IS E1 RC AT 41

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

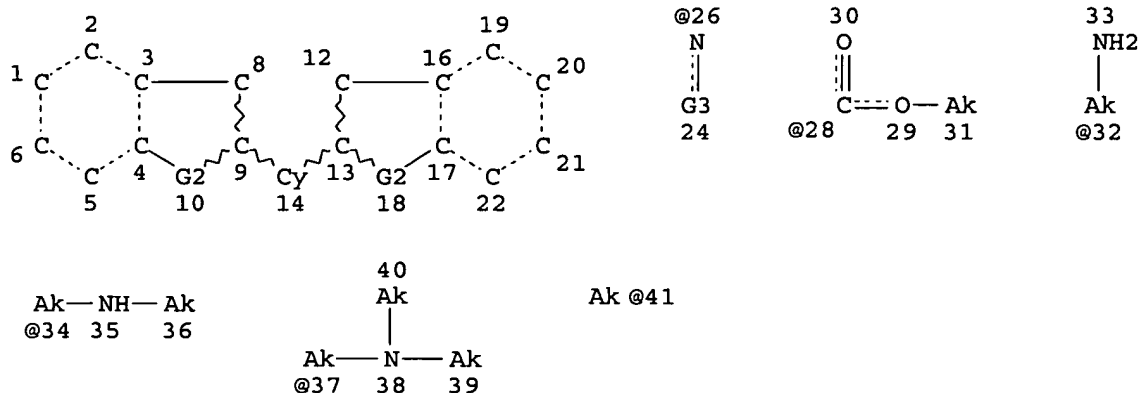
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L16 65882 SEA FILE=REGISTRY SSS FUL L14

L17 STR



```

VAR G2=N/26
VAR G3=41/28/32/34/37
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  31
CONNECT IS E2  RC AT  32
CONNECT IS E2  RC AT  34
CONNECT IS E1  RC AT  36
CONNECT IS E2  RC AT  37
CONNECT IS E1  RC AT  39
CONNECT IS E1  RC AT  40
CONNECT IS E1  RC AT  41
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

```

```

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  35

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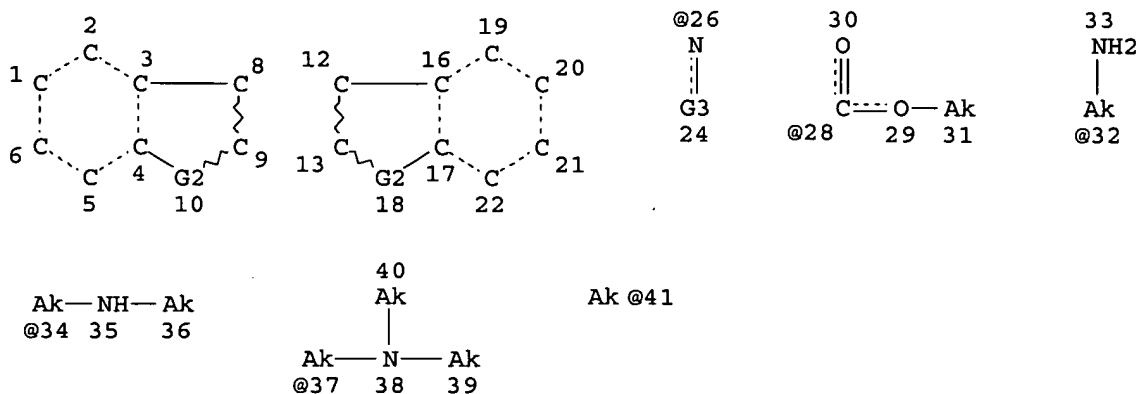
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STEREO ATTRIBUTES: NONE
L19          155 SEA FILE=REGISTRY SUB=L16 SSS FUL L17

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```
=> d que 122
```

```
L14          STR
```



```

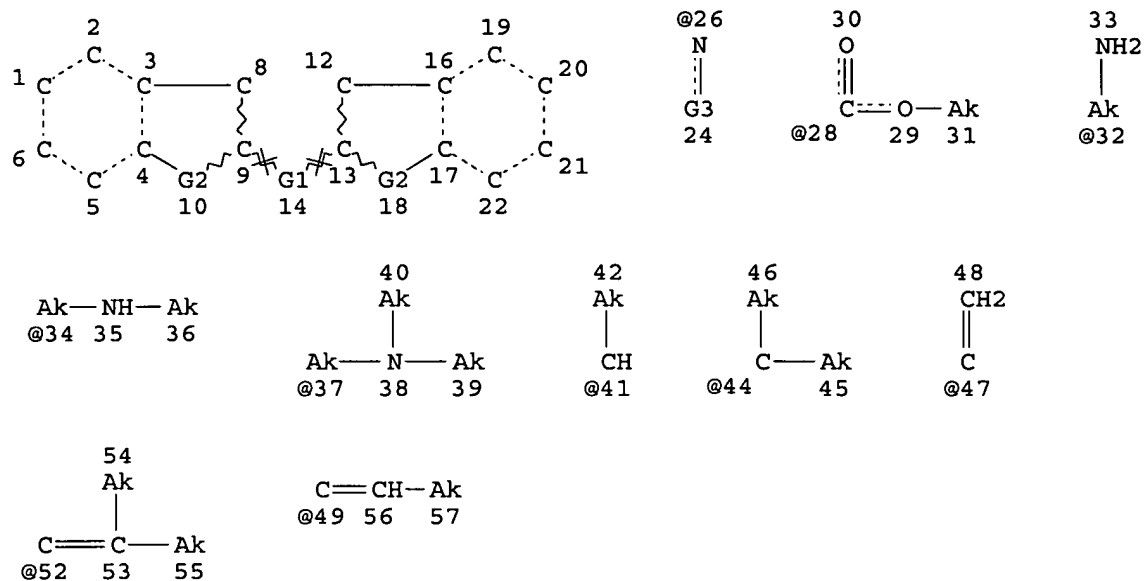
VAR G2=NH/26
VAR G3=41/28/32/34/37
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  31
CONNECT IS E2  RC AT  32
CONNECT IS E2  RC AT  34
CONNECT IS E1  RC AT  36

```

CONNECT IS E2 RC AT 37
 CONNECT IS E1 RC AT 39
 CONNECT IS E1 RC AT 40
 CONNECT IS E1 RC AT 41
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
 L16 65882 SEA FILE=REGISTRY SSS FUL L14
 L20 STR

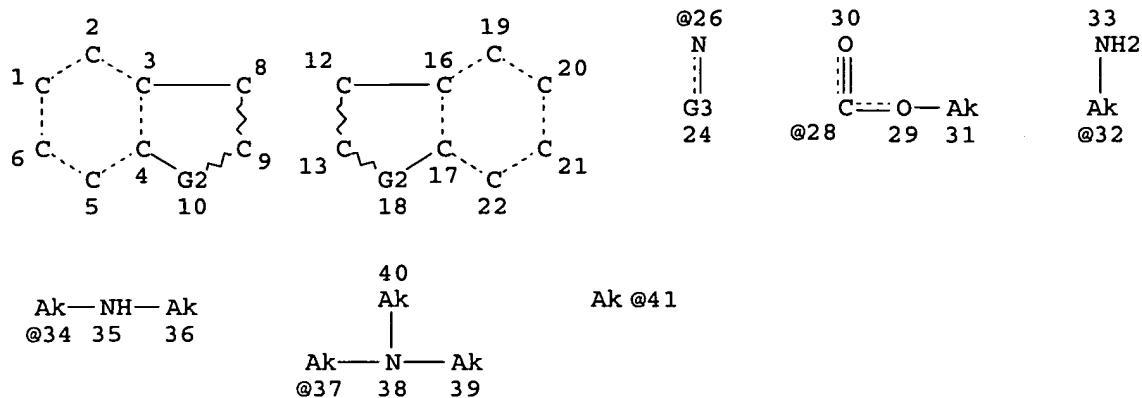


VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N
 VAR G2=NH/26
 VAR G3=AK/28/32/34/37
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE
 L22 623 SEA FILE=REGISTRY SUB=L16 SSS FUL L20

=> d que l32
 L14 STR



VAR G2=NH/26

VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 31

CONNECT IS E2 RC AT 32

CONNECT IS E2 RC AT 34

CONNECT IS E1 RC AT 36

CONNECT IS E2 RC AT 37

CONNECT IS E1 RC AT 39

CONNECT IS E1 RC AT 40

CONNECT IS E1 RC AT 41

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

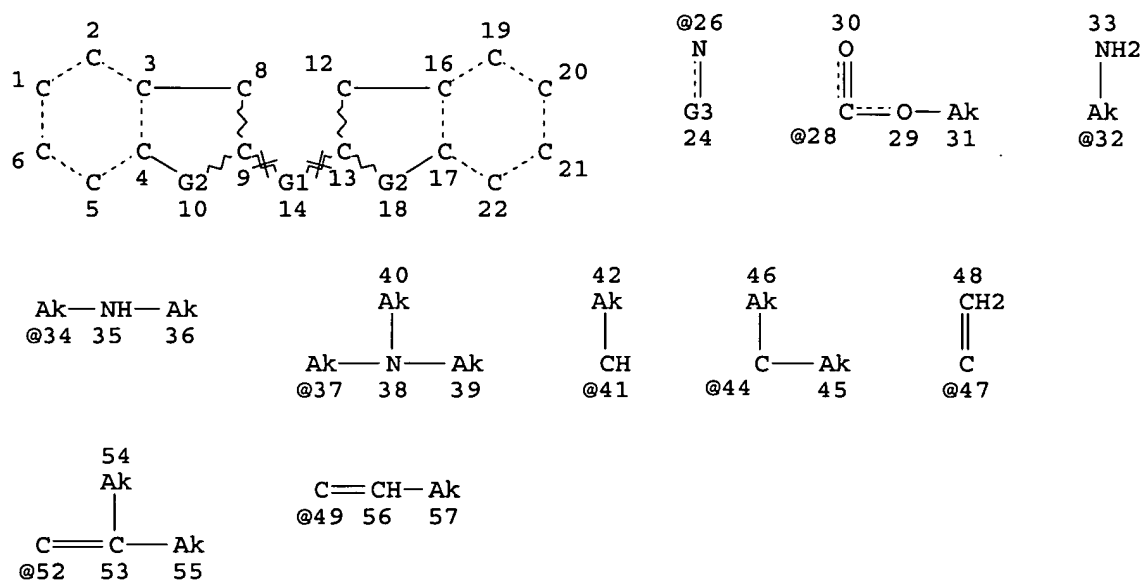
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L16 65882 SEA FILE=REGISTRY SSS FUL L14

L20 STR



VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

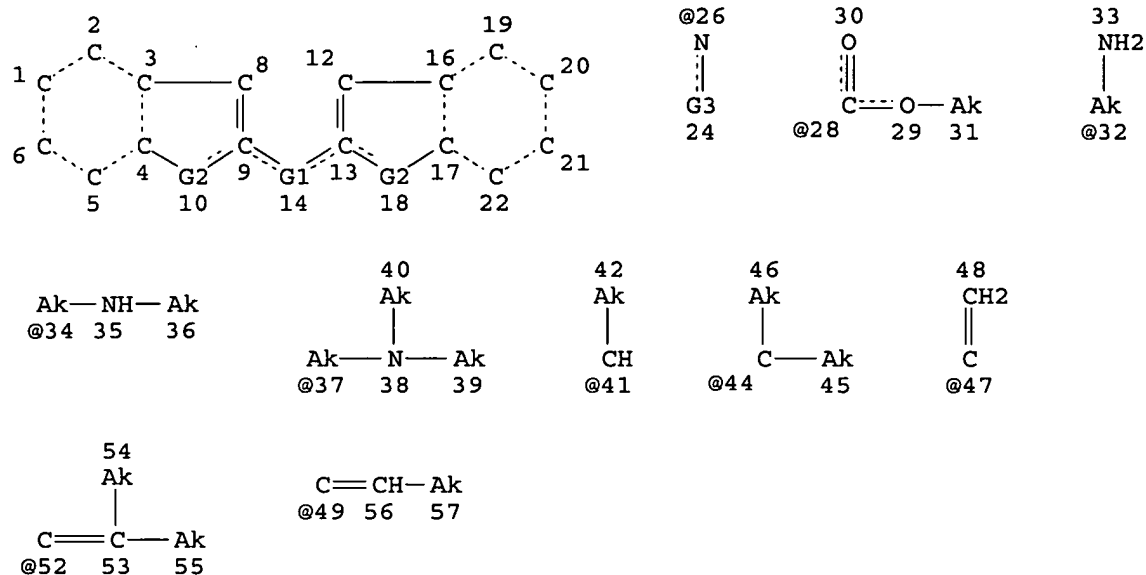
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L22 623 SEA FILE=REGISTRY SUB=L16 SSS FUL L20

L30 STR



VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 1

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 5

CONNECT IS M1 RC AT 6

CONNECT IS M1 RC AT 8

CONNECT IS M1 RC AT 12

CONNECT IS M1 RC AT 19

CONNECT IS M1 RC AT 20

CONNECT IS M1 RC AT 21

CONNECT IS M1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

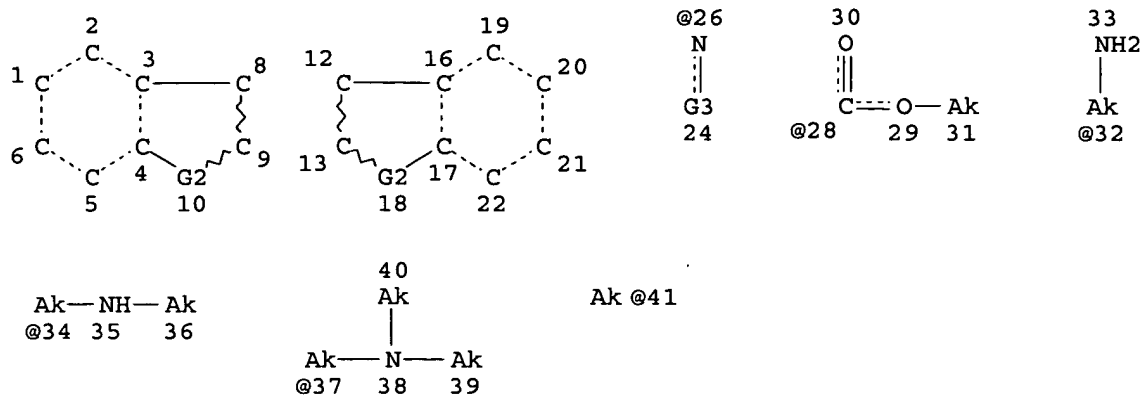
NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L32 82 SEA FILE=REGISTRY SUB=L22 CSS FUL L30

=> d que 138

L14 STR



VAR G2=NH/26

VAR G3=41/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 31

CONNECT IS E2 RC AT 32

CONNECT IS E2 RC AT 34

CONNECT IS E1 RC AT 36

CONNECT IS E2 RC AT 37

CONNECT IS E1 RC AT 39

CONNECT IS E1 RC AT 40

CONNECT IS E1 RC AT 41

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

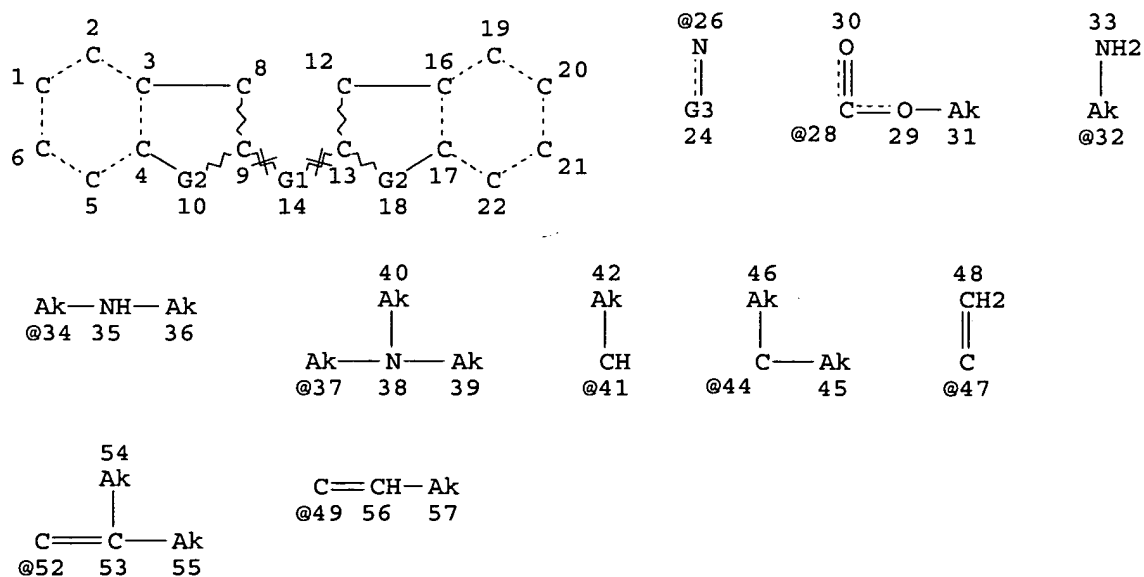
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L16 65882 SEA FILE=REGISTRY SSS FUL L14

L20 STR



VAR G1=O/S/CH2/41/44/47/49/52/NH/26/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

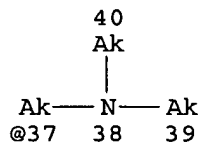
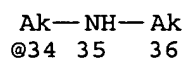
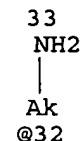
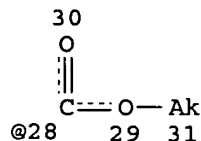
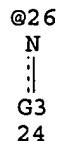
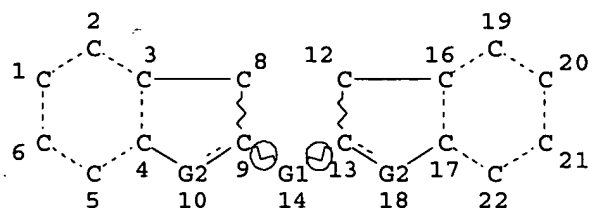
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

L22 623 SEA FILE=REGISTRY SUB=L16 SSS FUL L20

L36 STR



VAR G1=O/S/C/N

VAR G2=NH/26

VAR G3=AK/28/32/34/37

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 1

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 5

CONNECT IS M1 RC AT 6

CONNECT IS M1 RC AT 8

CONNECT IS M1 RC AT 12

CONNECT IS M1 RC AT 19

CONNECT IS M1 RC AT 20

CONNECT IS M1 RC AT 21

CONNECT IS M1 RC AT 22

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L38 109 SEA FILE=REGISTRY SUB=L22 SSS FUL L36

=> d his

(FILE 'HOME' ENTERED AT 06:32:46 ON 24 FEB 2005)

SET COST OFF

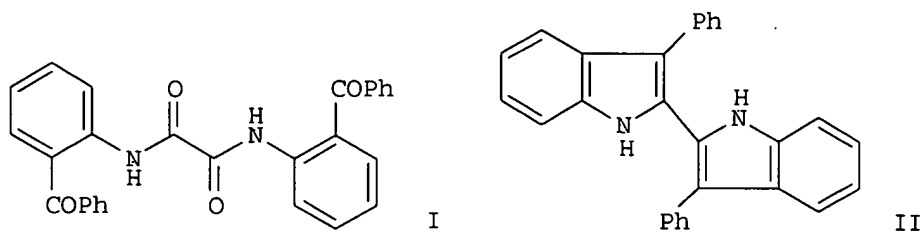
FILE 'REGISTRY' ENTERED AT 06:33:00 ON 24 FEB 2005

L1 STR

L2 1 S L1 CSS SAM

FILE 'HCAPLUS' ENTERED AT 06:41:34 ON 24 FEB 2005

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:505286 CAPLUS
 DOCUMENT NUMBER: 123:83146
 TITLE: Titanium-induced zipper reactions
 AUTHOR(S): Fuerstner, Alois; Ptock, Arne; Weintritt, Holger; Goddard, Richard; Krueger, Carl
 CORPORATE SOURCE: Max-Planck-Inst. Kohlenforschung, Muelheim an der Ruhr, D-45470, Germany
 SOURCE: Angewandte Chemie, International Edition in English (1995), 34(6), 678-81
 CODEN: ACIEAY; ISSN: 0570-0833
 PUBLISHER: VCH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 123:83146
 GI



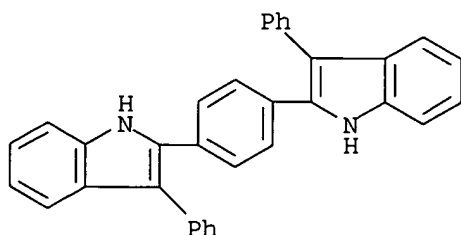
AB A one step titanium-induced zipper reaction results in an amazing and unprecedented chemo- and regioselectivity in the reductive cyclization of polycarbonyl compds. Thus, polycarbonyl compound I was treated with TiCl_3 and zinc dust under argon to give 80% biindole derivative II.

IT 164936-88-3P 164936-89-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (titanium-induced zipper reactions)

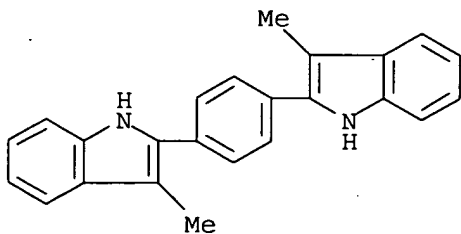
RN 164936-88-3 CAPLUS

CN 1H-Indole, 2,2'-(1,4-phenylene)bis[3-phenyl- (9CI) (CA INDEX NAME)

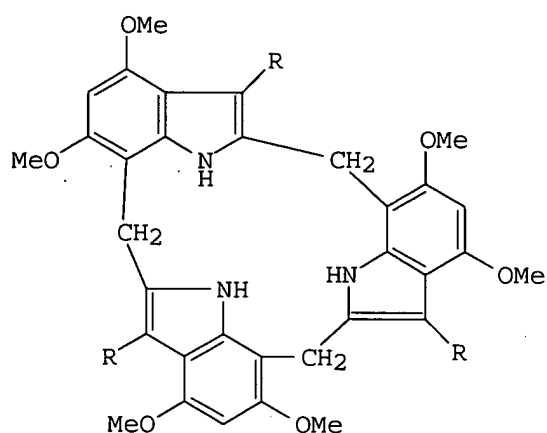


RN 164936-89-4 CAPLUS

CN 1H-Indole, 2,2'-(1,4-phenylene)bis[3-methyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1993:671129 CAPLUS
 DOCUMENT NUMBER: 119:271129
 TITLE: Calix[3]indoles, new macrocyclic
 tris(indolylmethylene) compounds with 2,7-linkages
 AUTHOR(S): Black, David S. C.; Bowyer, Michael C.; Kumar, Naresh;
 Mitchell, Peter S. R.
 CORPORATE SOURCE: Sch. Chem., Univ. New South Wales, Kensington, 2033,
 Australia
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1993), (10), 819-21
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 119:271129
 GI



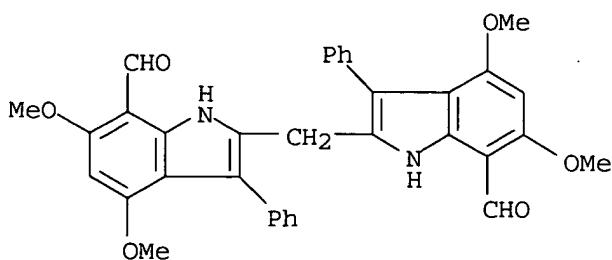
AB A series of macrocyclic tris(indolylmethylene) compds., e.g. I [R = (un)substituted Ph], can be obtained from 7- or 2-(hydroxymethyl)indoles or from the combination of either an indole with a bis(hydroxymethyl)-2,7'-diindolylmethane or a bis(hydroxymethyl)indole with a 2,7'-diindolylmethane; an isomeric series can be obtained from the combination of an indole with a bis(hydroxymethyl)-2,2'-diindolylmethane.

IT 151321-09-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reduction of)

RN 151321-09-4 CAPLUS

CN 1H-Indole-7-carboxaldehyde, 2,2'-methylenebis[4,6-dimethoxy-3-phenyl-(9CI) (CA INDEX NAME)



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1987:617419 CAPLUS
 DOCUMENT NUMBER: 107:217419
 TITLE: Reactivity and reaction paths of methyl-substituted
 bis(indolylcarbenium) ions
 AUTHOR(S): Pindur, Ulf; Mueller, Johann
 CORPORATE SOURCE: Fachbereich Pharm., Univ. Mainz, Mainz, D-6500, Fed.
 Rep. Ger.
 SOURCE: Journal of Heterocyclic Chemistry (1987), 24(1),
 159-63
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 107:217419
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

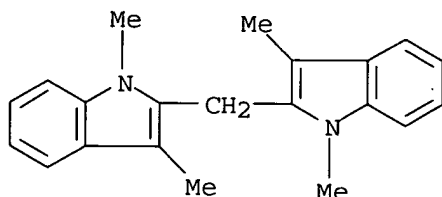
AB Me substituted bisindolylcarbenium ions I and II (R = H, Me) react with
 some O- and C-nucleophiles regioselectively. The cations II yield with
 hydroxide ions the tetraindolyldimethyl ether III and with methoxide ions
 the bisindolylmethoxymethanes IV. I and II react with several
 methylindoles to give isomeric bis- and trisindolylmethanes. An
 electrophilic reactivity order of cations I and II can be derived from the
 exptl. results.

IT **91455-03-7P 110968-29-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

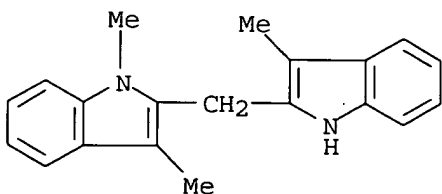
RN 91455-03-7 CAPLUS

CN 1H-Indole, 2,2'-methylenebis[1,3-dimethyl- (9CI) (CA INDEX NAME)

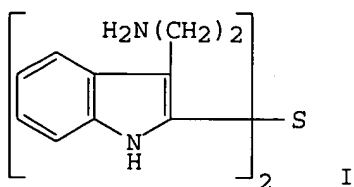


RN 110968-29-1 CAPLUS

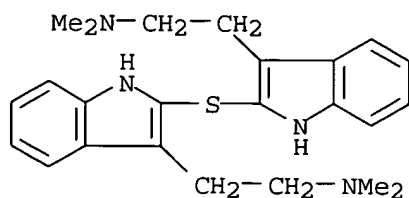
CN 1H-Indole, 1,3-dimethyl-2-[(3-methyl-1H-indol-2-yl)methyl]- (9CI) (CA
 INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1985:184940 CAPLUS
 DOCUMENT NUMBER: 102:184940
 TITLE: A novel serotonin antagonist 2,2'-bis[3-(2-N,N-dimethylaminoethyl)indolyl]sulfide (BDIS)
 AUTHOR(S): Chu, C. K.; Wander, J. D.; Tackett, R. L.; Iturrian, W. B.; Schmitz, J. P.; Garner, G. E.; Chae, K.
 CORPORATE SOURCE: Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA
 SOURCE: Journal of Heterocyclic Chemistry (1984), 21(6), 1901-3
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
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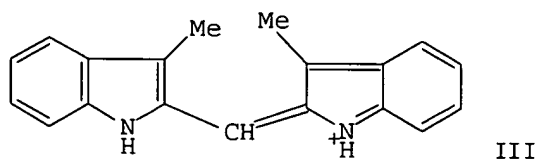
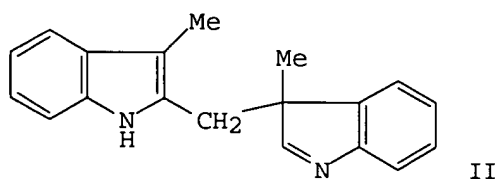
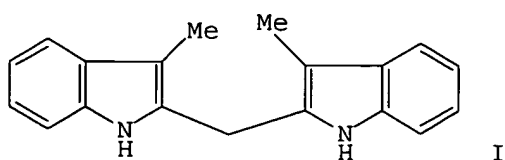


AB A novel serotonin antagonist, 2,2'-bis[3-(2-N,N-dimethylaminoethyl)indolyl]sulfide (I) was synthesized in 1 step from the reaction of N,N-dimethyltryptamine with SO₂Cl₂.
 IT **96249-78-4P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 96249-78-4 CAPLUS
 CN 1H-Indole-3-ethanamine, 2,2'-thiobis[N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1980:471451 CAPLUS
 DOCUMENT NUMBER: 93:71451
 TITLE: 2,3'-Bis(3-methylindolyl)methane from 3-methylindole
 and formaldehyde
 AUTHOR(S): Brieskorn, Carl Heinz; Huber, Johannes
 CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Wuerzburg,
 Wuerzburg, D 8700, Fed. Rep. Ger.
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1979),
 312(12), 1046-51
 CODEN: ARPMAS; ISSN: 0365-6233
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI



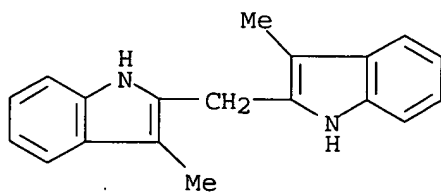
AB Hopkins-Cole reaction of 3-methylindole with H₂CO in MeOH-H₂SO₄ gave I and II. II is the precursor of ion III, the color product of this reaction.

IT **36798-17-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 36798-17-1 CAPLUS

CN 1H-Indole, 2,2'-methylenebis[3-methyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:111897 CAPLUS

DOCUMENT NUMBER: 82:111897

TITLE: Reaction of skatole with iodine in the presence of thiourea

AUTHOR(S): Hino, Tohru; Endo, Mamoru; Nakagawa, Masako

CORPORATE SOURCE: Fac. Pharm. Sci., Chiba Univ., Chiba, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1974), 22(11), 2728-31

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

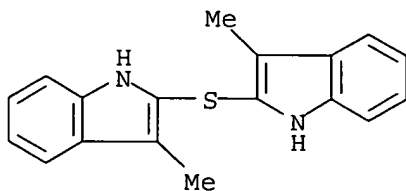
AB Skatole was treated with iodine and H₂NCSNH₂ in EtOH containing KI to give the indoles I (11.6%), II (23%), and III (13%), 3.4% 3-methyloxindole, 3-methyldioxindole (trace), and 2.2% bis(3-methyl-2-indolyl) sulfide. I also was prepared by treating 2-bromoskatole with H₂N-CSNH₂-HBr followed by KI.

IT 55132-21-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55132-21-3 CAPLUS

CN 1H-Indole, 2,2'-thiobis[3-methyl- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:59818 CAPLUS

DOCUMENT NUMBER: 80:59818

TITLE: Preparation of 3-substituted 2-indolinethiones via diindolyl disulfides. Reaction of 3-substituted indoles with sulfur monochloride

AUTHOR(S): Hino, Tohru; Suzuki, Toshikazu; Takeda, Sachie; Kano, Nobuko; Ishii, Yoichi; Sasaki, Akira; Nakagawa, Masako
CORPORATE SOURCE: Fac. Pharm. Sci., Chiba Univ., Chiba, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1973), 21(12), 2739-48

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

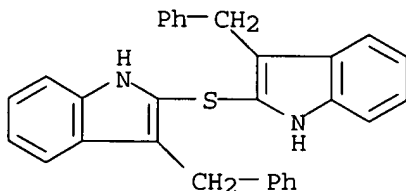
AB The reaction of 3-alkylindoles (I) with S₂Cl₂ in ether gave the corresponding 2-diindolyl disulfides (II, n = 2) as the main product, and mono- and trisulfides (I, n = 1,3) as minor products. The similar reaction of 3-arylindoles gave the disulfides in good yields. Reduction of the diindolyl disulfides with NaBH₄ in EtOH afforded the 2-indolinethiones (III) in good yields.

IT 51206-69-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of, indolinethiones by)

RN 51206-69-0 CAPLUS

CN 1H-Indole, 2,2'-thiobis[3-(phenylmethyl)- (9CI) (CA INDEX NAME)



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1972:405277 CAPLUS
 DOCUMENT NUMBER: 77:5277
 TITLE: Light-induced reactions of α -(N-alkylanilino) ketones. Formation of diindolylmethanes
 AUTHOR(S): Hill, J.; Townend, J.
 CORPORATE SOURCE: Dep. Chem., Univ. Salford, Salford, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1210-19
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Irradiation of 6 α -(N-alkylanilino) ketones, $\text{PhN}(\text{CH}_2\text{R})\text{CHR}_1\text{C(OMe)}$ (I; R, R_1 = H, Me, or Ph), in MeOH, Me_2CHOH , or benzene caused fission of the α C-N bond giving a secondary amine (PhNHCH_2R), a ketone ($\text{R}_1\text{CH}_2\text{C(OMe)}$), an α -[p-(alkylamino)phenyl] ketone formed by para rearrangement, and a substituted 2-methylindole formed by ortho rearrangement with subsequent cyclodehydration. I (R_1 = H) also gave a diindol-3-ylmethane derived from the 2-methylindole. Irradiation of I with 1,2-dimethylindole gave diindolylmethanes, via 1-phenylazetidinols as labile intermediates. Irradiation of 7 anilino ketones $\text{PhNRCH}_2\text{COR}_1$ (R = H, Me, or Me_3C ; R_1 = Me, Et, Me_3C , or Ph) was also studied.
 IT **36798-56-8P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 36798-56-8 CAPLUS
 CN 1H-Indole, 2,2'-methylenebis[3-ethyl-1-methyl- (9CI) (CA INDEX NAME)]

